Teaching PROFESSOR new math

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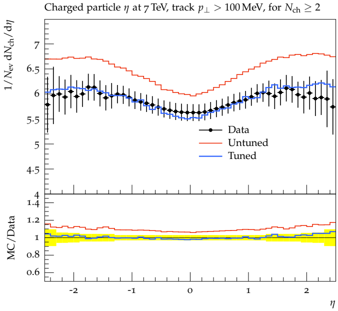
MPI@LHC 2018 Perugia, 13 December 2018

Tuning

- Goal: best possible physics prediction of MC generator
- Realistic events contain physics at low scales where perturbation breaks down
- Rely on model assumptions that introduce many parameters
- Need to find “meaningful” settings
- Can be done manually but hard to do on a reasonable time-scale because of MC run-time and dimensionality of problem

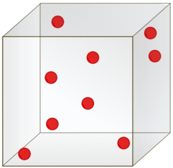


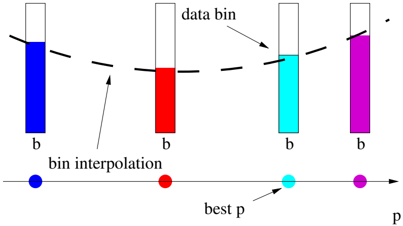
Tuning with Professor in a nutshell

- Random sampling: N parameter points in n-dimensional space
- Run generator and fill histograms (e.g. Rivet) trivial parallel
- Polynomial approximation *per bin*
- Construct goodness-of-fit measure

$$\phi^2(\vec{p}) = \sum_b w_b^2 \cdot \frac{(f_b(\vec{p}) - \mathcal{R}_b)^2}{\Delta^2}$$

- and numerically *minimise* with `iminuit`





In the following this will be called the “inner optimisation” problem

Inner and outer optimisation

- Incompatible datasets and mismodelling in MC generator necessitate introduction of tuning weights w_b
- Adjusting the weights has so far been a manual procedure
- The user would iteratively run the "inner optimisation" and look at resulting plots
- We propose an automated procedure for this "outer optimisation":
  - Write goodness-of-fit in terms of histograms/observables
  - The parameter space is now the observable-weight space
  - Inner optimisation yields best fit point, $\hat{p}$, for given

$$\{w_{\mathcal{O}}\}$$

$$\sum_{\mathcal{O}=1}^{N} w_{\mathcal{O}}^2 \cdot \sum_{b\in\mathcal{O}} \frac{(f_b(\vec{p}) - \mathcal{R}_b)^2}{\Delta^2} \xrightarrow[\text{yields}]{\text{Minimisation}} \boxed{\hat{p}|\{w_{\mathcal{O}}\}}$$

- $\hat{p}$ is used to evaluate an objective function for the outer optimisation

Portfolio objective

- For given $\hat{p}$, we can calculate the per-observable goodness-of fit

$$\nu_{\mathcal{O}}(\hat{p}|\{w_{\mathcal{O}}\}) = \frac{1}{N_{\text{bins}}(\mathcal{O})} \sum_{b\in\mathcal{O}} \frac{(f_b(\hat{p}|\{w_{\mathcal{O}}\}) - \mathcal{R}_b)^2}{\Delta^2}, \ \mathcal{O} = 1, \ldots, N$$

- With N such measures, we can calculate mean and standard deviation (dropped argument $\hat{p}|\{w_{\mathcal{O}}\}$for readability)

$$\mu = \frac{1}{N} \sum_{\mathcal{O}=1}^{N} \nu_{\mathcal{O}}$$

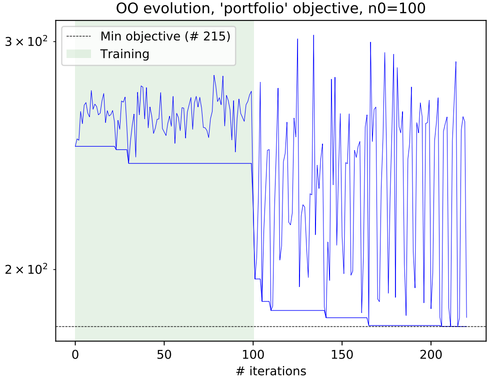
$$\sigma^2 = \frac{1}{N} \sum_{\mathcal{O}=1}^{N} [\nu_{\mathcal{O}} - \mu]^2$$

- And construct an objective function to minimise

$$\min_{w_{\mathcal{O}}\in[0,1]} \lambda \cdot \mu(\hat{p}|\{w_{\mathcal{O}}\}) + \sigma^2(\hat{p}|\{w_{\mathcal{O}}\}), \quad \text{s.t.} \ \sum_{\mathcal{O}=1}^{N} w_{\mathcal{O}} = 1.$$

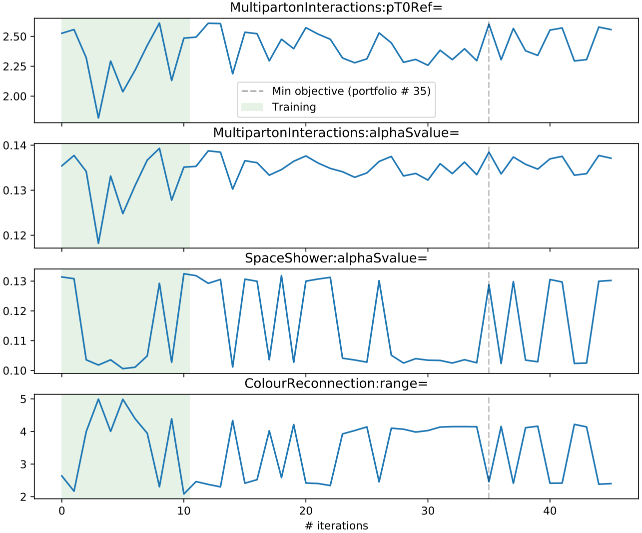
Outer optimisation

- Minimisation of portfolio objective is iterative, gradient free
- We train a radial basis function (RBF) and use it to walk through the weight space
- RBF minimisation alternates between local and global search
- Convergence is fast but depends on initial guess → multi-start approach (that's ok since inner optimisation is really fast)



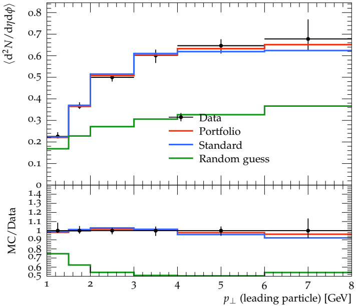
Evolution of inner optimisation

- This plot shows the $\hat{p}$ of the inner optimisation
- Shows the correlation of parameters

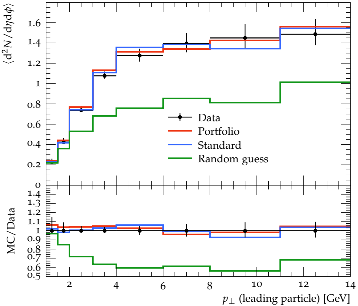


Comparison of results

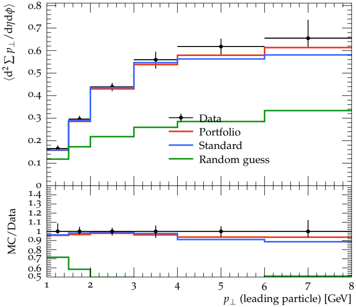
Transverse N density vs. $p_\perp^{\text{clus1}}$, $\sqrt{s} = 900$ GeV



Transverse N density vs. $p_\perp^{\text{clus1}}$, $\sqrt{s} = 7$ TeV



Transverse $\sum p_\perp$ density vs. $p_\perp^{\text{clus1}}$, $\sqrt{s} = 900$ GeV



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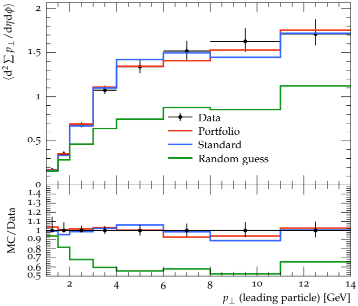
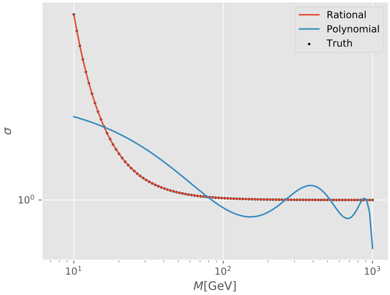
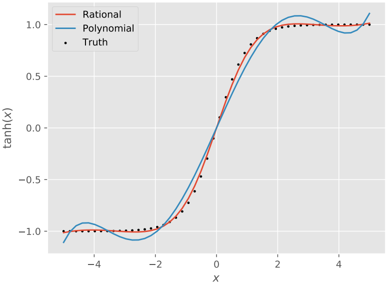


Rational approximation

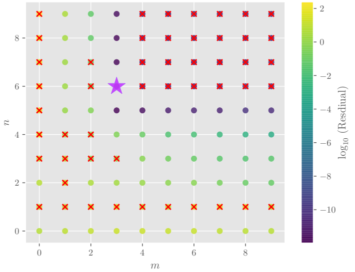
- Polynomial approximation does not capture $1/x$ behaviour well
- E.g. masses in propagators, MPI cut-off
- $\rightarrow$ Multivariate rational approximation $f(\vec{p}) = g(\vec{p})/h(\vec{p})$
- With g, h being polynomials of order m, n
- N.b. polynomials are limit where $h(\vec{p})$ is constant ($n = 0$)

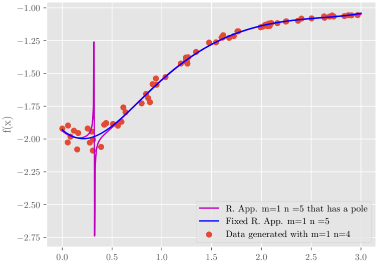




Spurious poles and selecting m and n

- Especially in presence of noisy data: spurious poles
- For numerical reasons, denominator polynomial can have roots
- Root finding greatly helped by knowledge of gradient
- We have a brute force and a smart method to deal with that:
  - Compute all possible approximations (m, n), pick the best without pole
  - Instead of linear algebra, use non-linear optimisation with constraints to solve $\|f(\vec{p})h(\vec{p}) - g(\vec{p})\|$, iteratively adding constraints on poles when found

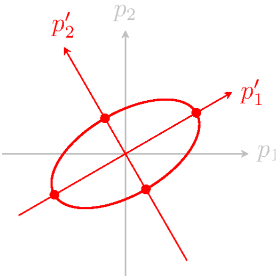


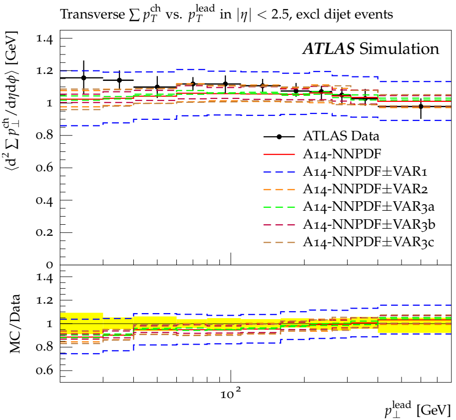


Tuning uncertainties (with A. Buckley)

So far: exploit minimiser covariance matrix in parameter space

- Linear algebra to find principal directions
- In each direction: find intercept with χ^2 contour
- Problem: $\Delta\chi^2 = 1$ recipe does not always work
- $\rightarrow$ Ad-hoc definition of $\Delta\chi^2$ by looking at plots (e.g. A14)

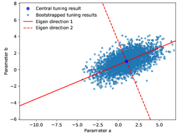


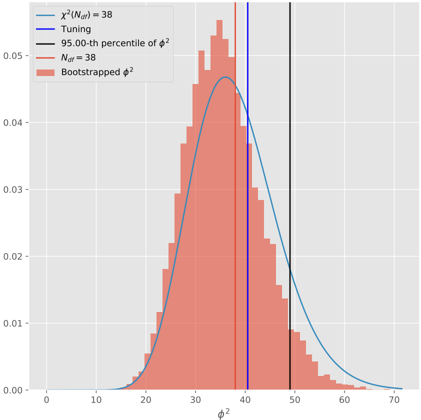


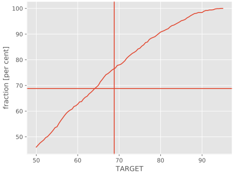
Bootstrapping the goodness-of-fit

To overcome the ad-hoc nature, obtain the actual distribution of the goodness-of-fit measure, Φ^2

- Tuning replicas — smear data within its uncertainies, run minimisation for each replica and record Φ^2



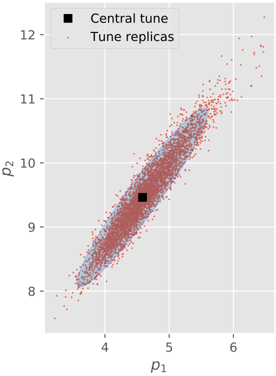


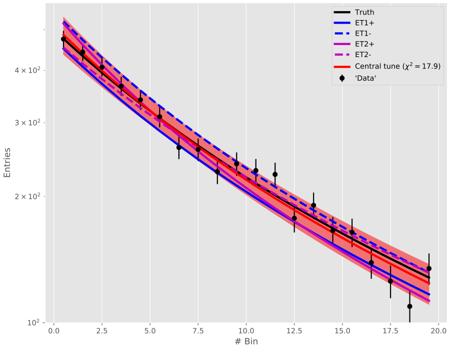


- Problem: coverage test revealed that there is a 25% chance the central tuning is outside the 68th percentile of Φ^2

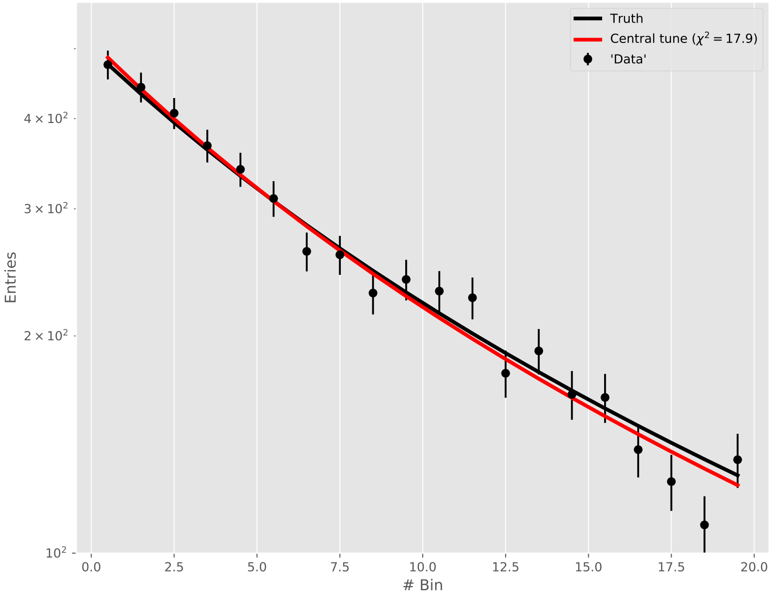
Latest attempt

- Still do the tuning replicas
- Forget about Φ^2, χ^2 values, forget about minimiser covariance
- Instead:
  - Calculate covariance in parameter space from tuning replicas
  - Linear algebra to find principal directions, eigenvalues for aspect ratio of ellipsoid
  - Find ellipsoid that contains 68.8% of tuning replicas
  - Intercept with principal axes gives “Eigentunes”





Construction



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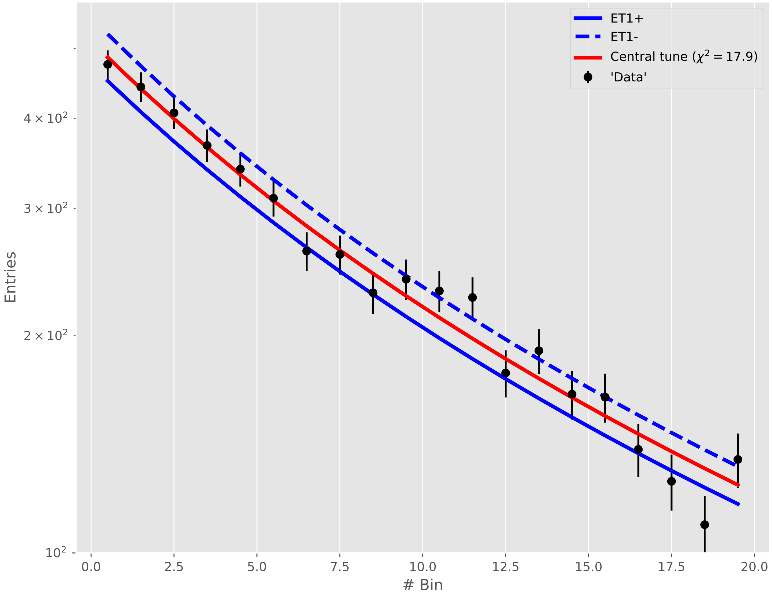

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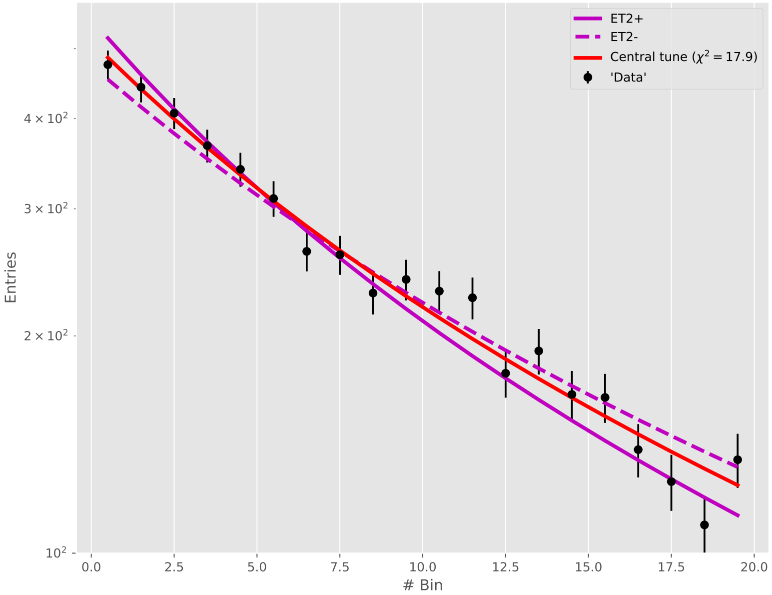

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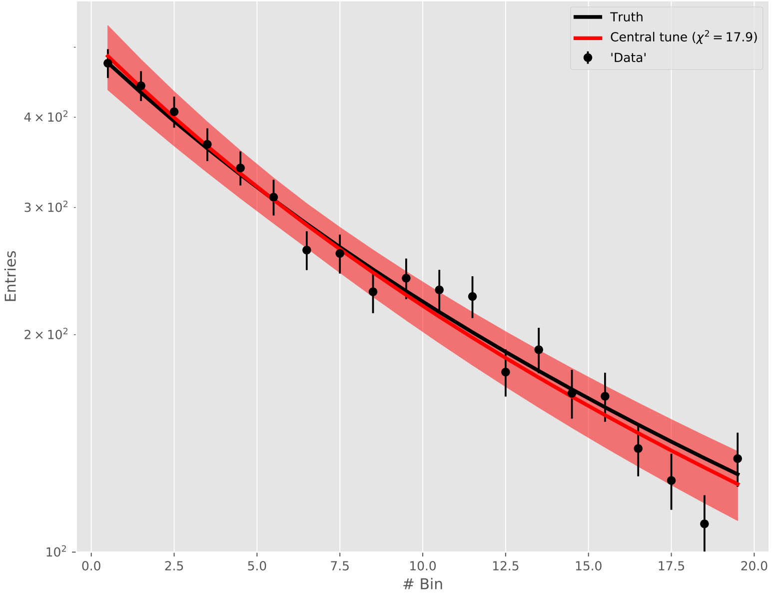

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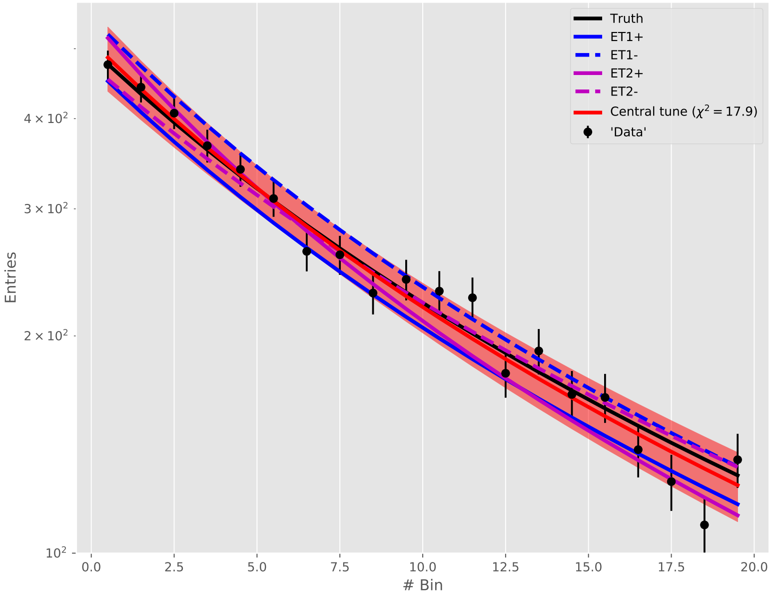

Summary

- Algorithm for a more automated tuning:
  - Outer optimisation loop in the weight space
  - Minimisation of portfolio objective function
- Algorithm for multivariate rational approximation
  - Rational approximation are a natural extension of polynomials used so far
  - Better quality interpolations
  - Spurious poles are a bit of a nuisance but can now be dealt with
- New suggestion to get tuning uncertainties
  - Tuning replicas through data smearing
  - Confidence ellipsoid construction and intercept with principal directions